Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Materials
for

Gaussian Approximation Potentials for Accurate Thermal Properties of Two-Dimensional Materials

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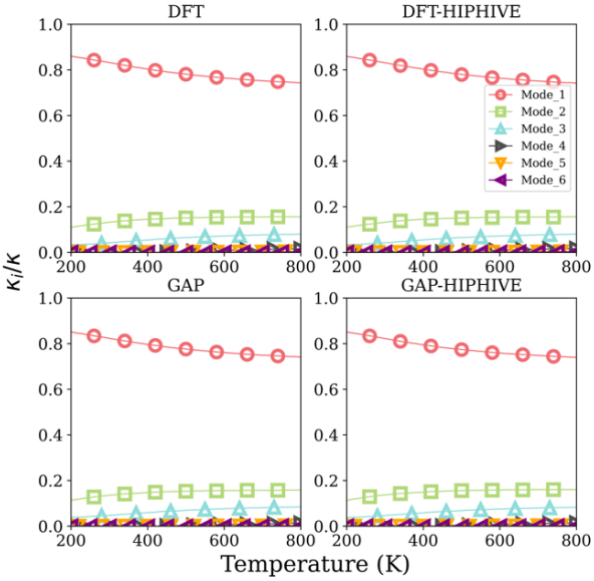
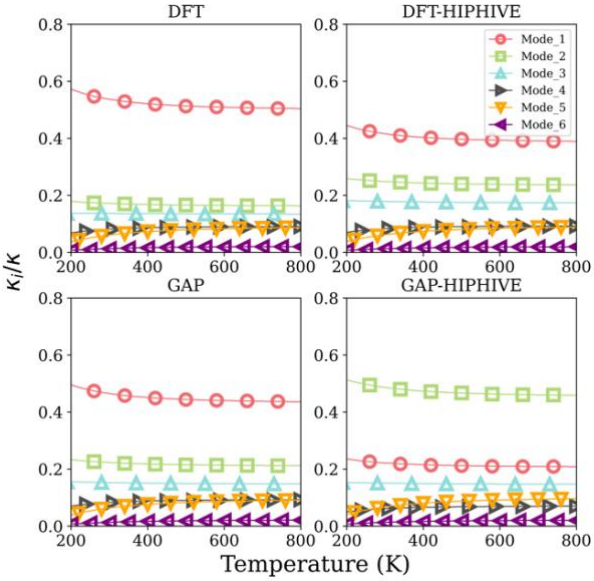
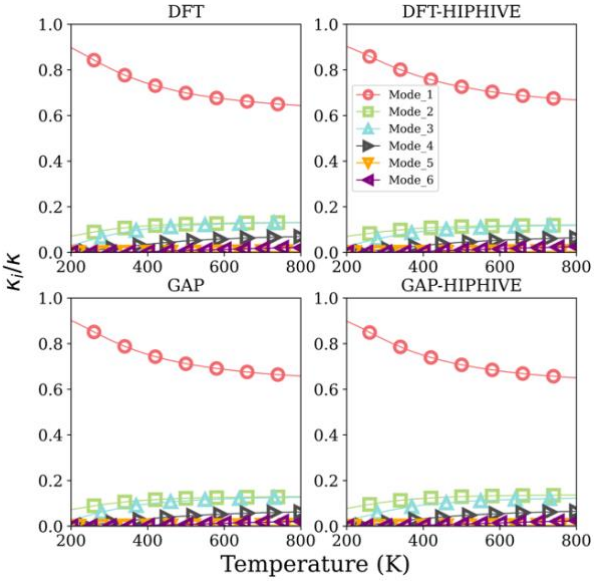
(a) Graphene



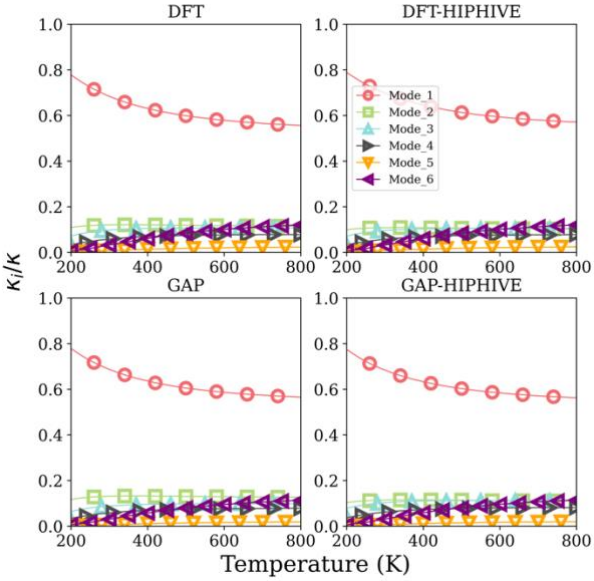
(b) Silicene



(c) *h*-BN



(d) *h*-AlN



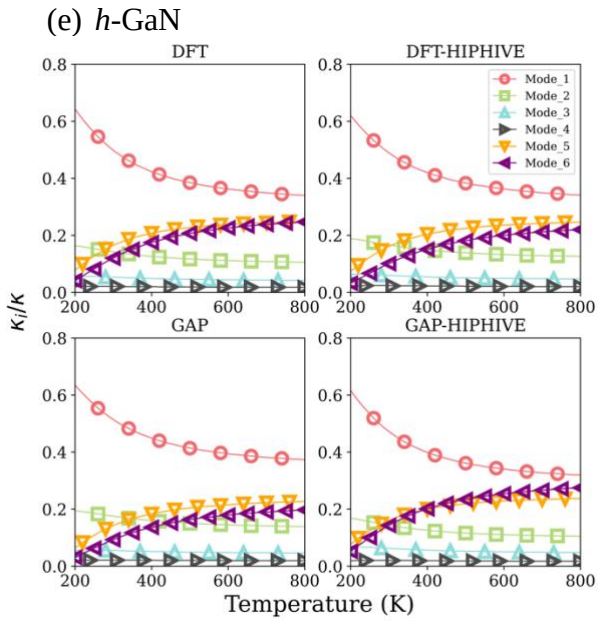
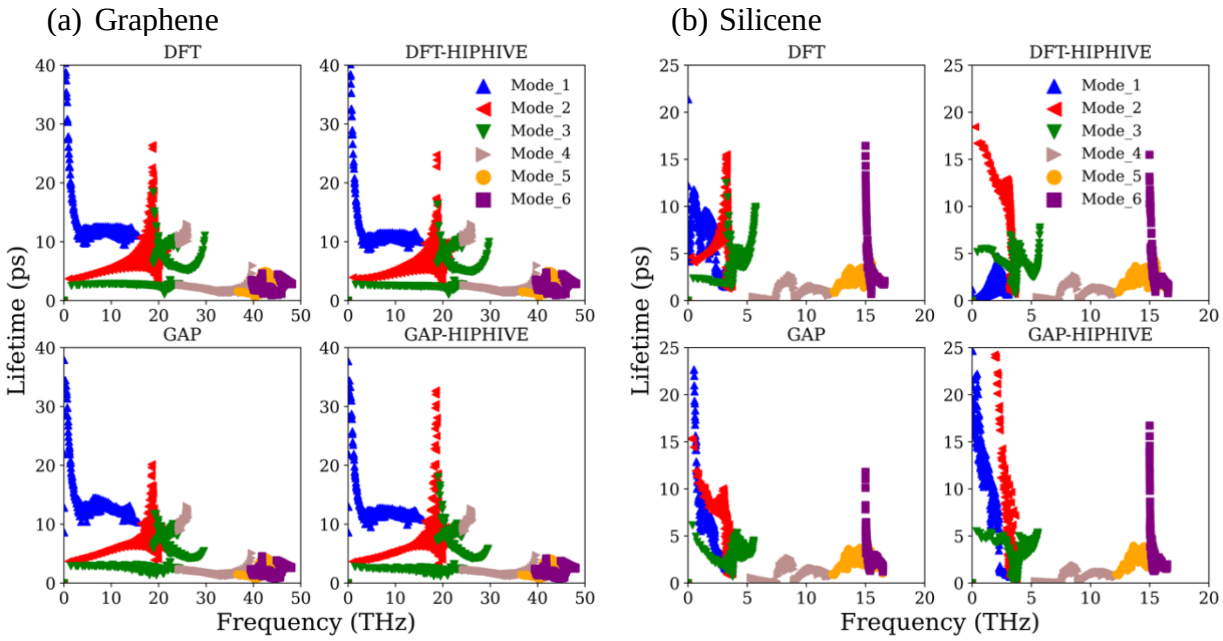


Figure S1: Normalized contribution of acoustic and optical phonon branches to the thermal conductivity as a function of temperature of all considered materials for DFT, GAP, DFT-HIPHIVE and GAP-HIPHIVE.



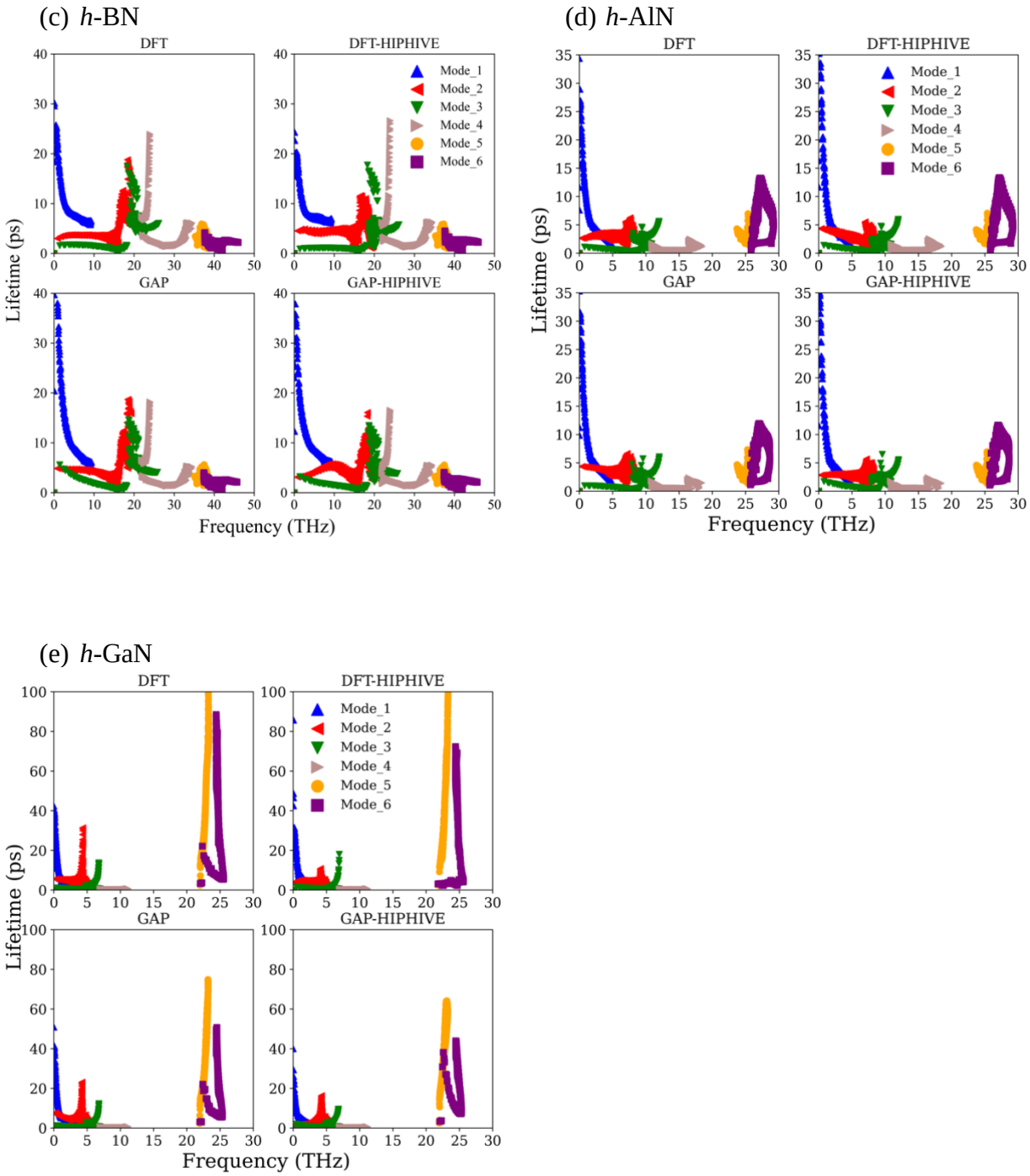
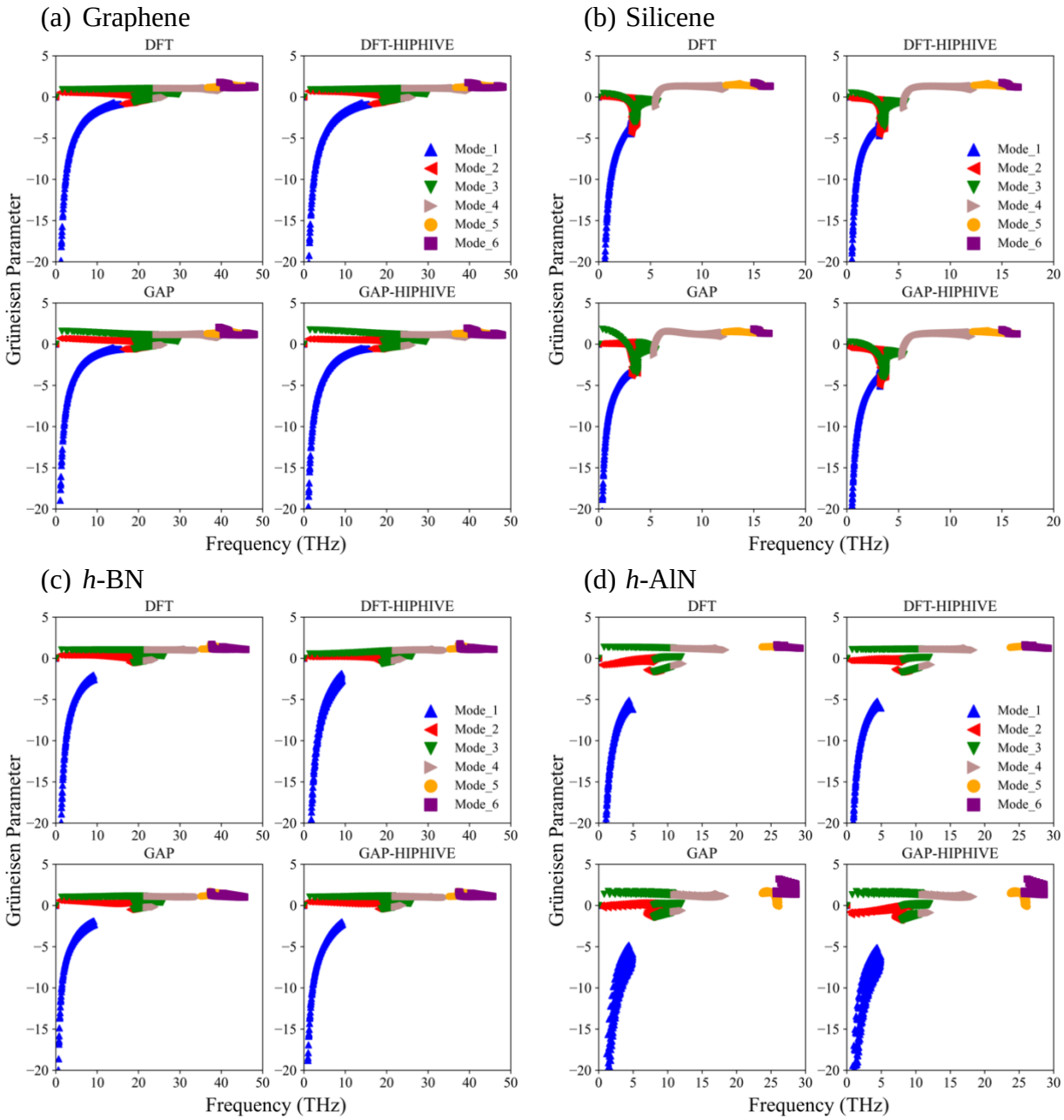


Figure S2: Relaxation time of phonon modes of all considered materials as a function of frequency for all phonon modes at T=300K for DFT, GAP, DFT-HIPHIVE, and GAP-HIPHIVE.


(a) Graphene
(b) Silicene
(c) h-BN
(d) h-AlN
DFT
DFT-HIPHIVE
GAP
GAP-HIPHIVE
Mode_1
Mode_2
Mode_3
Mode_4
Mode_5
Mode_6
Grüneisen Parameter
Frequency (THz)

(e) *h*-GaN

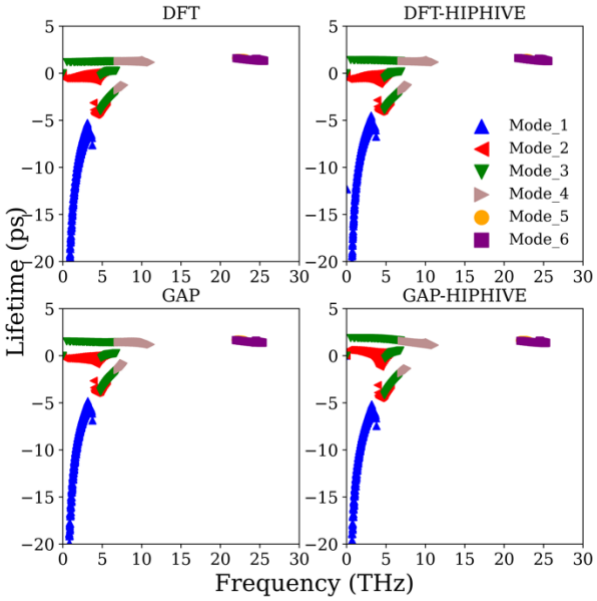
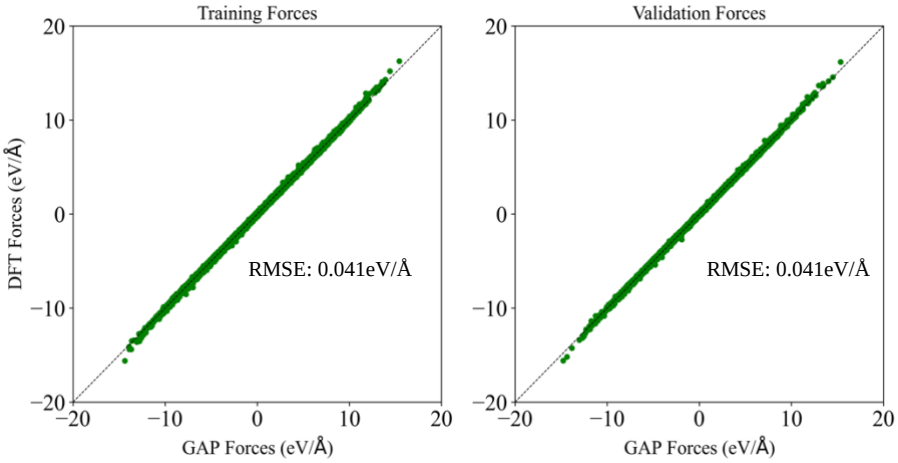
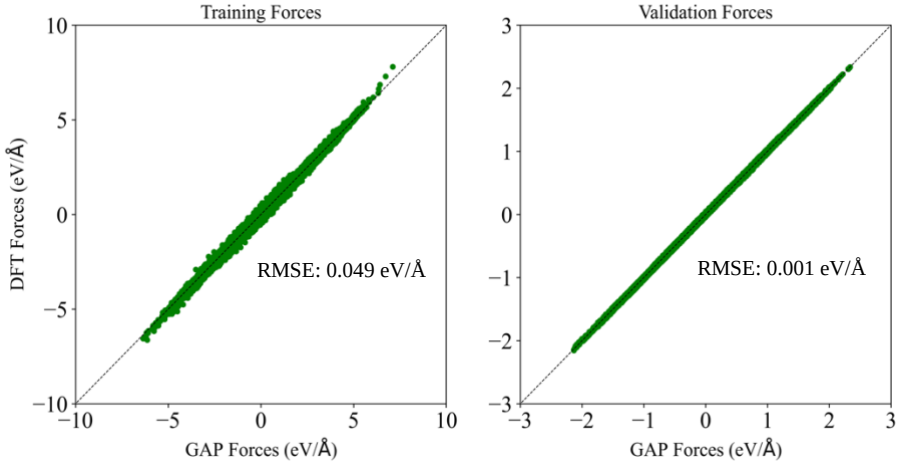


Figure S3: Grüneisen parameters as a function of the frequency of all considered materials.

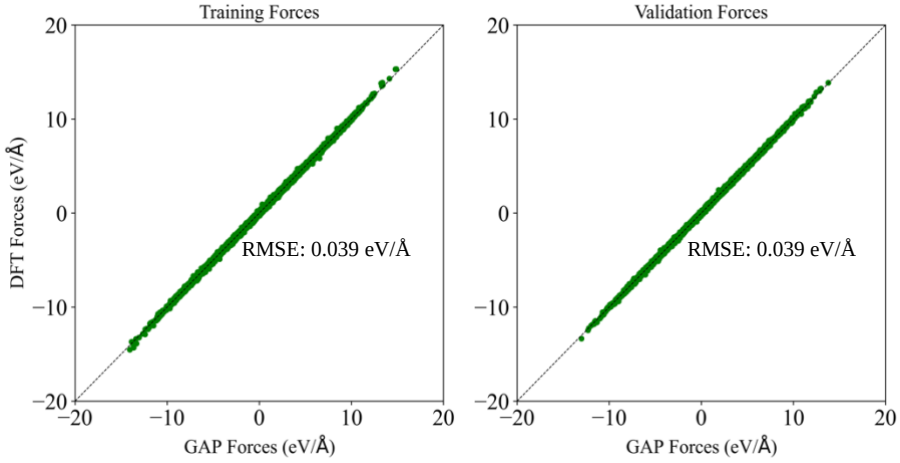
(a) Graphene



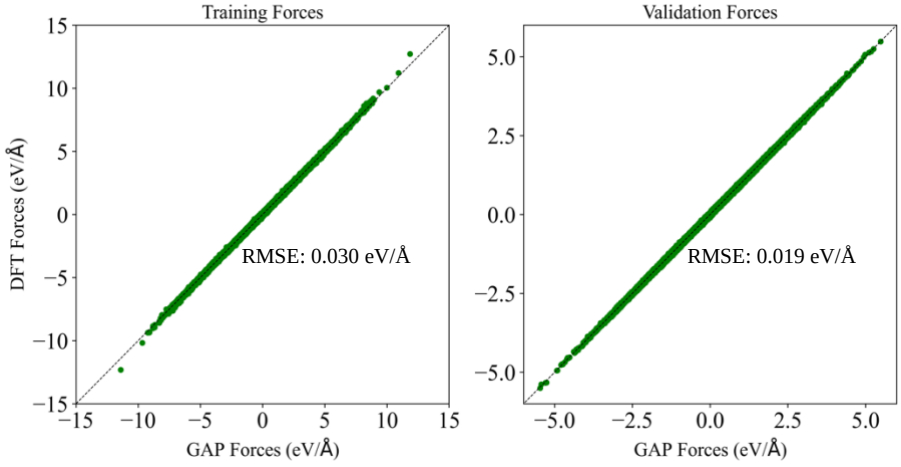
(b) Silicene



(c) *h*-BN



(d) *h*-AlN



(e) *h*-GaN

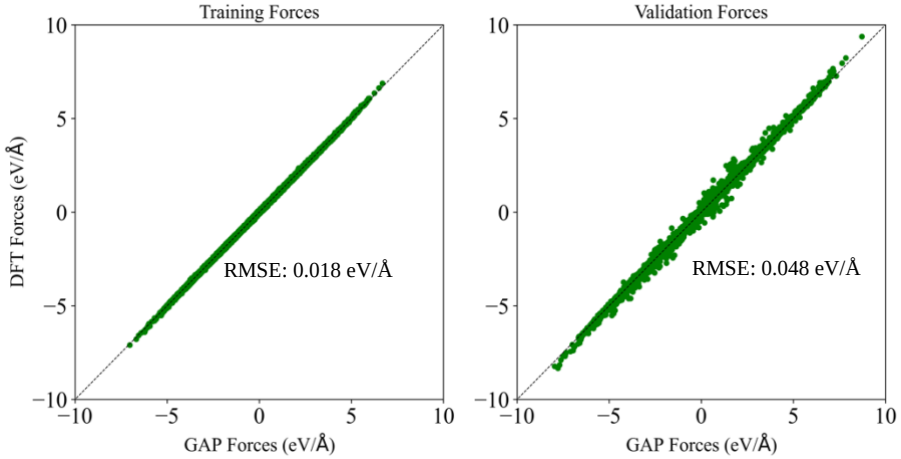
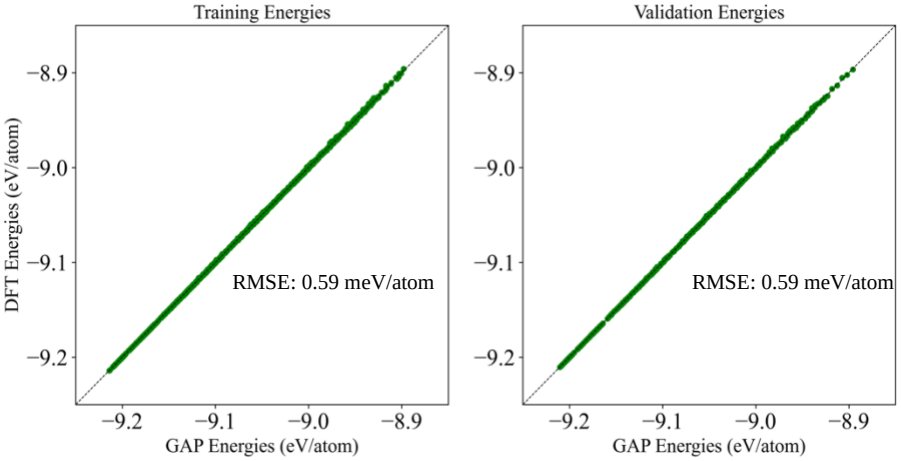
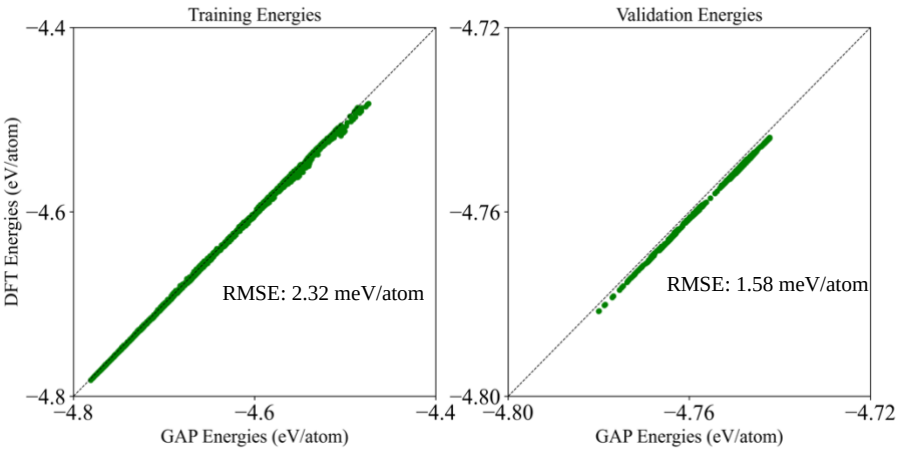


Figure S4: The comparison of forces on atoms between obtained by DFT and GAP

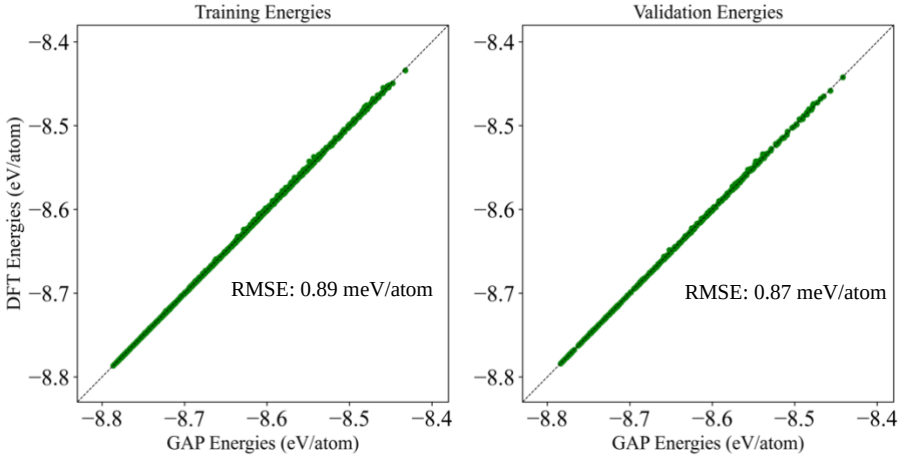
(a) Graphene



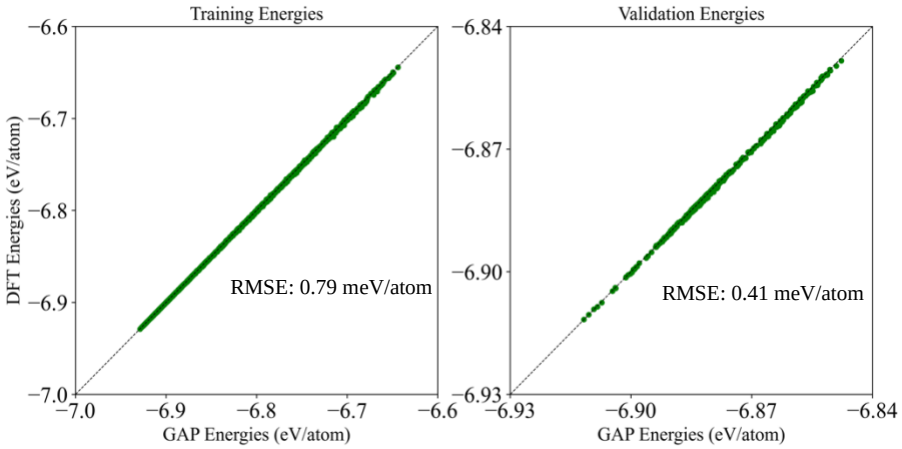
(b) Silicene



(c) *h*-BN



(d) *h*-AlN



(e) *h*-GaN

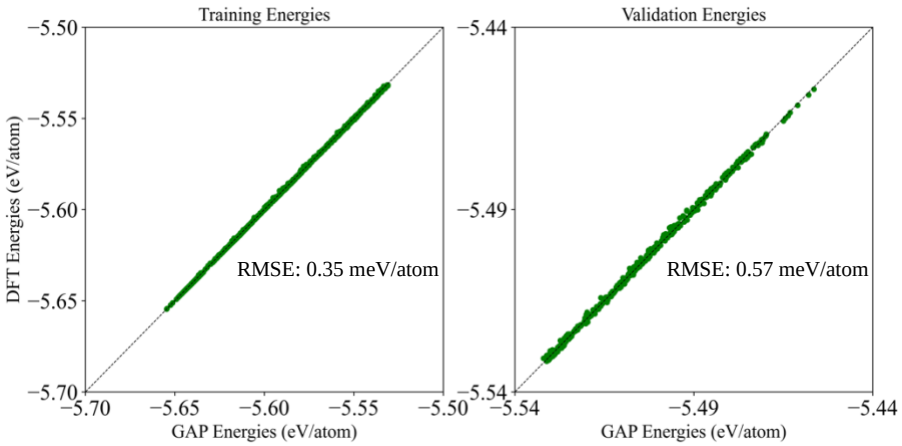


Figure S5: The comparison of energies between obtained by DFT and GAP

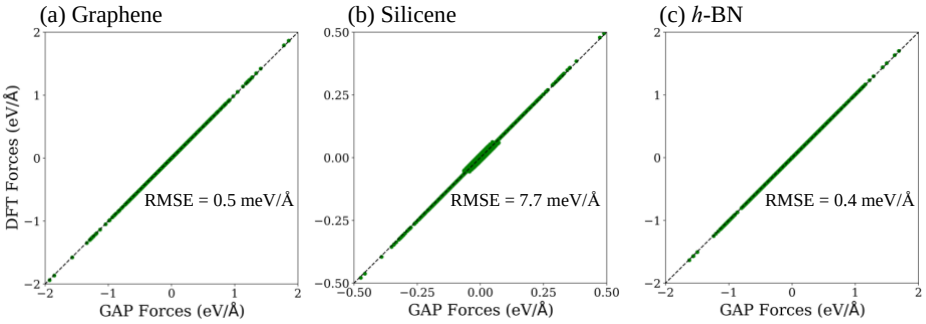
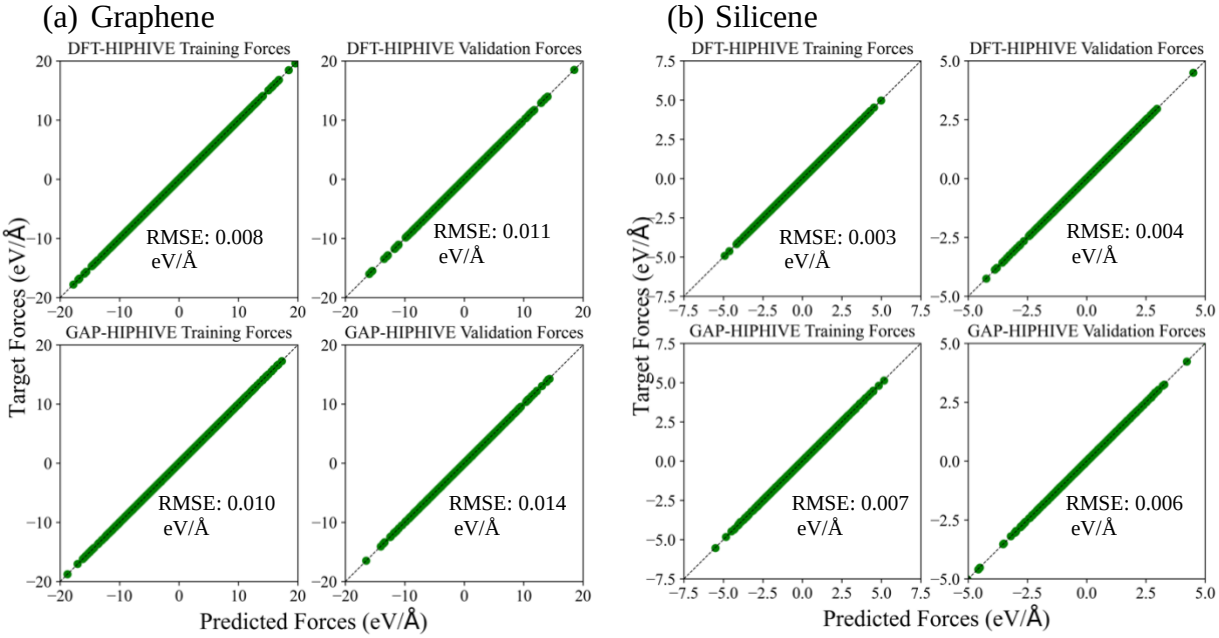


Figure S6: The comparison of the resulting interatomic forces due to the 4th order displacements, obtained by DFT and GAP.



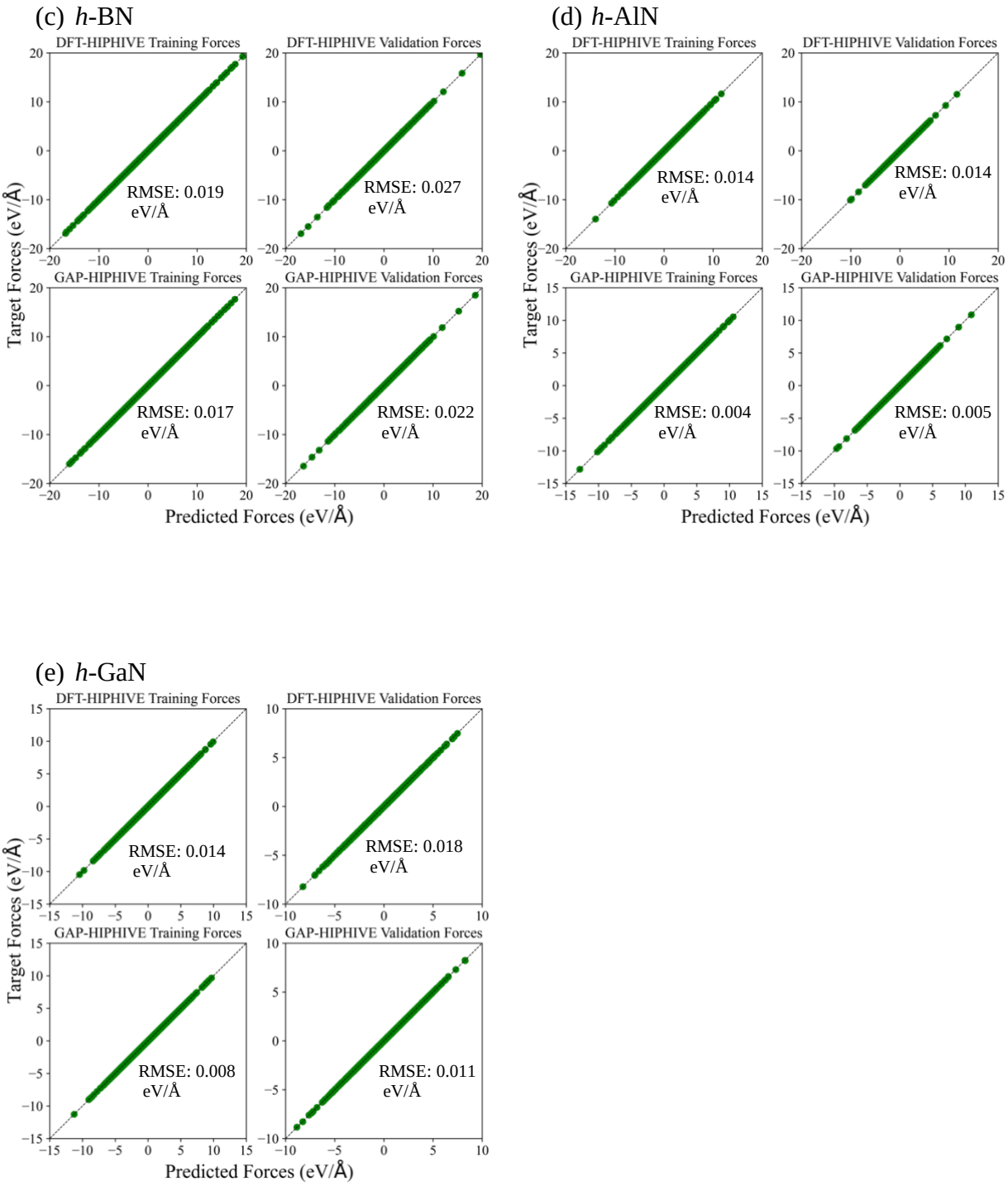
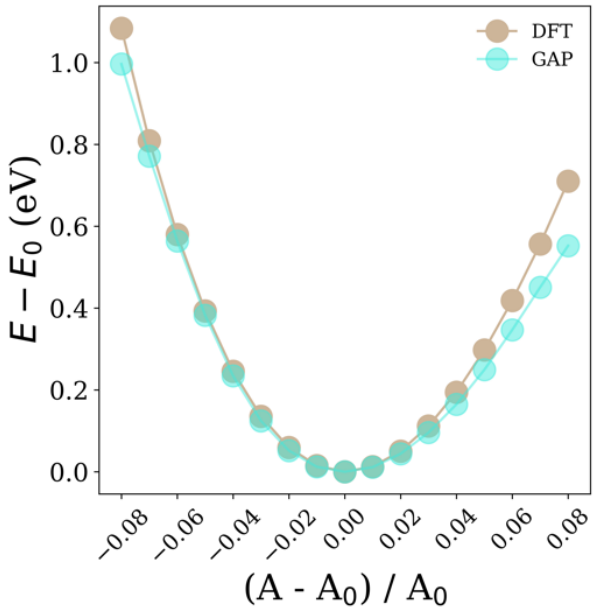
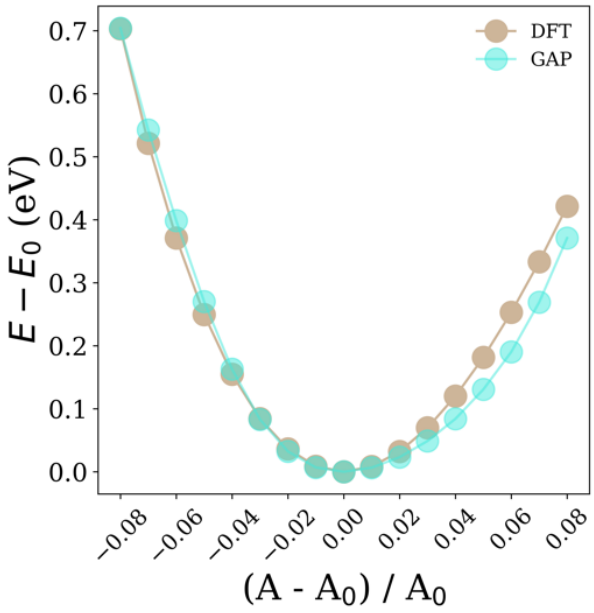


Figure S7: The comparison of forces on atoms between obtained by DFT (target) and HIPHIVE (predicted)

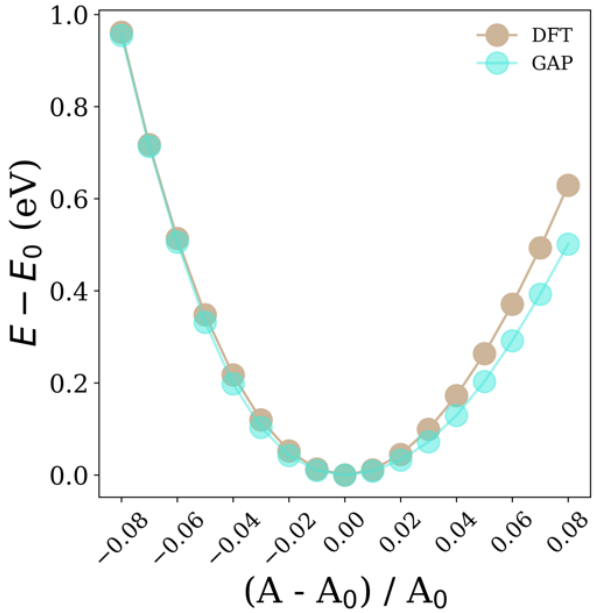
(a) Graphene



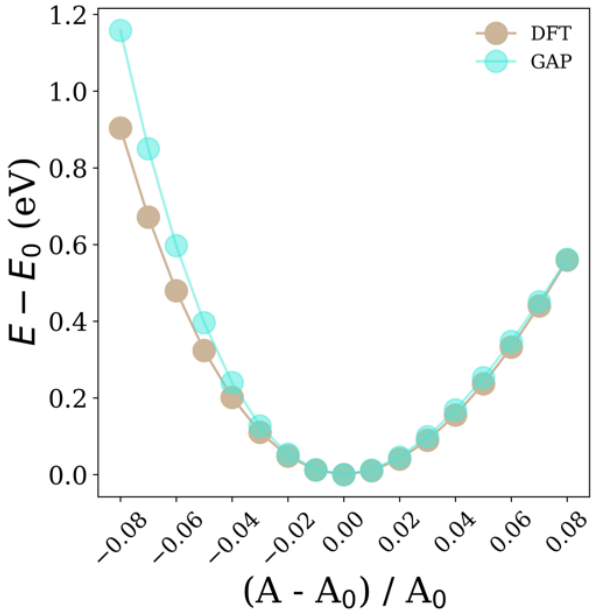
(b) Silicene



(c) *h*-BN



(d) *h*-AlN



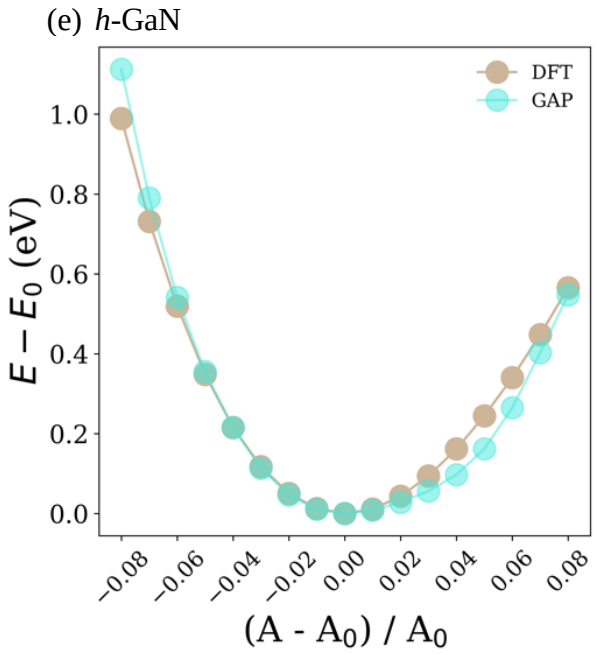


Figure S8: Variation of the system's total energy versus the relative difference of the cross-sectional area of the unit cell for all considered materials.

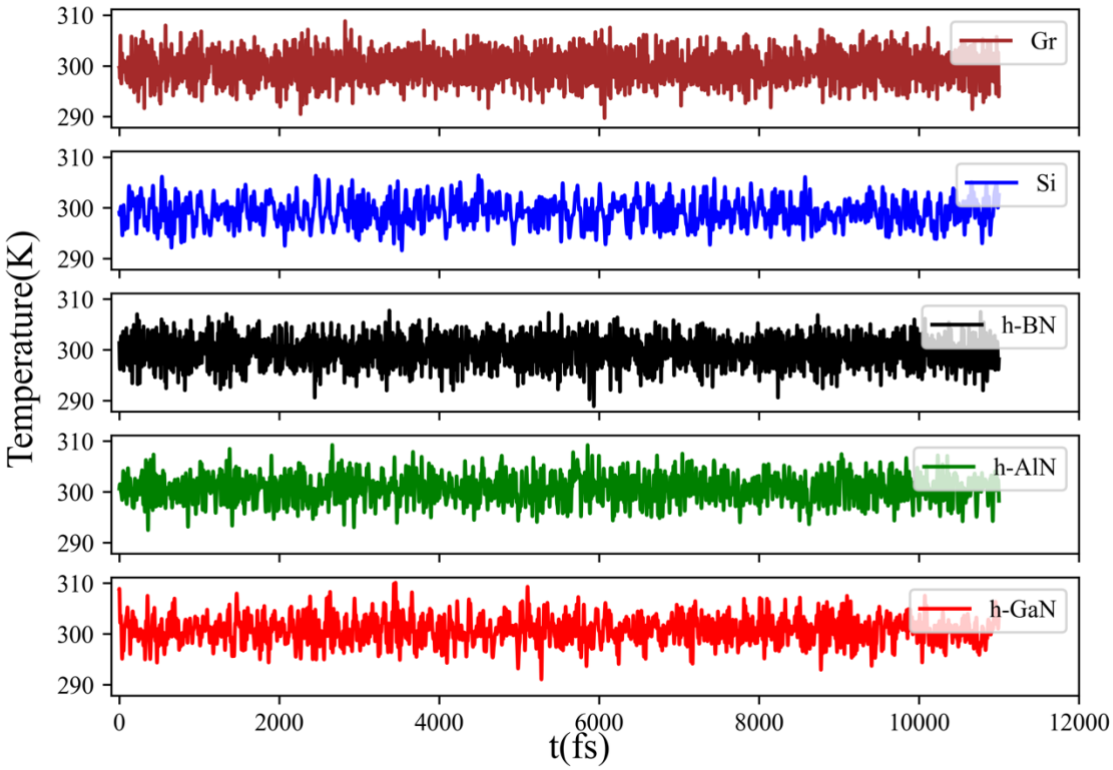


Figure S9: Time evolution of temperature fluctuation in the MD simulations at T = 300 K for all the considered materials.

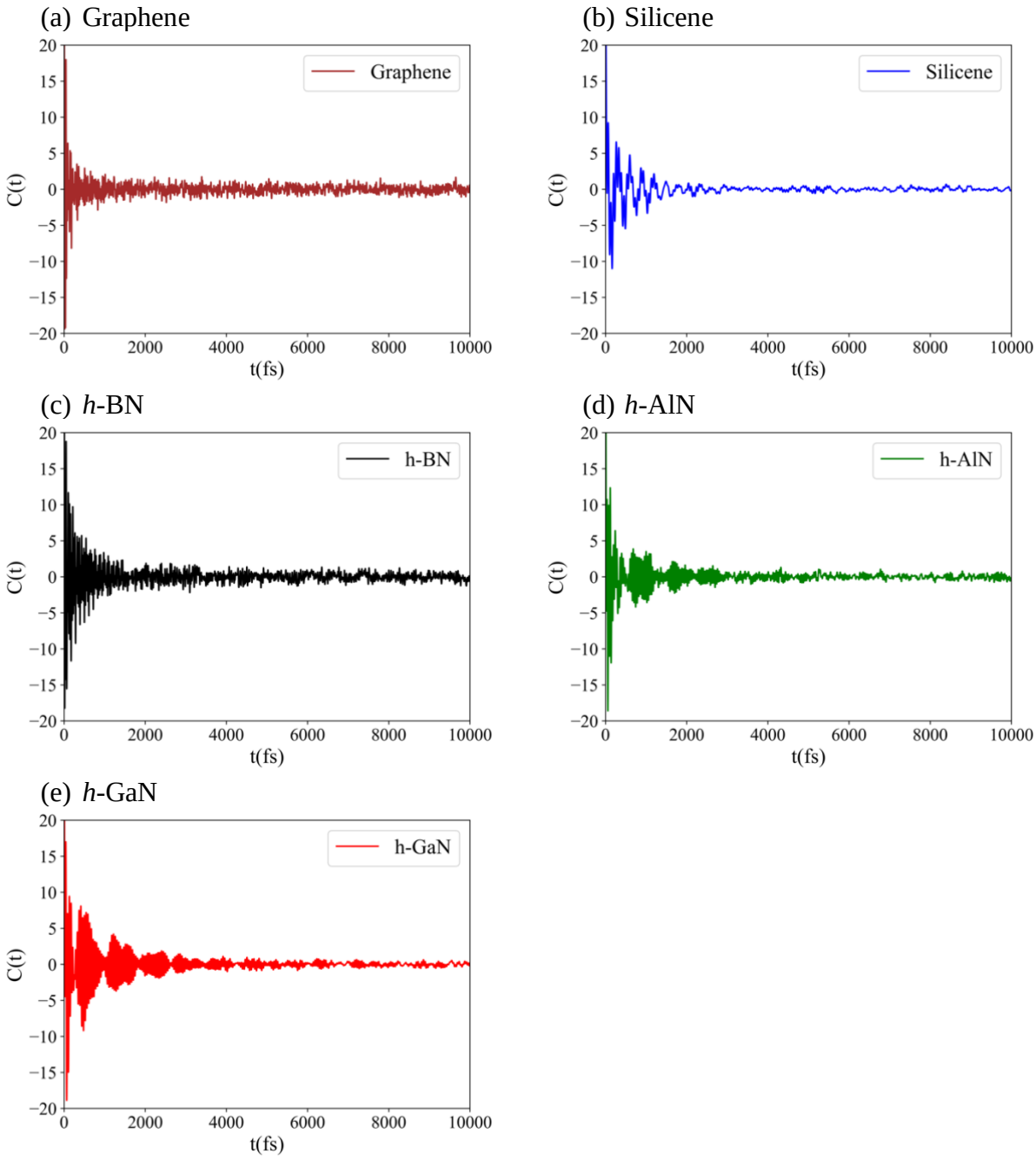


Figure S10: Velocity autocorrelation functions for all considered materials.

Table S1: Hyperparameters of all considered materials for the training of GAP.

Gr		Si		*h*-BN		*h*-AlN		*h*-GaN	
SOAP		SOAP		SOAP		SOAP		SOAP	
l_max	10	l_max	12	l_max	6	l_max	8	l_max	6
n_max	8	n_max	10	n_max	6	n_max	8	n_max	8
cutoff	5.2	cutoff	7.2	cutoff	6	cutoff	5.2	cutoff	7.2
sigma	0.4	sigma	0.5	sigma	0.4	sigma	0.5	sigma	0.4
zeta	4	zeta	4	zeta	2	zeta	4	zeta	2
n_sparse	1500	n_sparse	2000	n_sparse	1000	n_sparse	1000	n_sparse	1500
delta	0.2	delta	0.3	delta	0.2	delta	0.2	delta	0.2
# of Training_data	1500	# of Training_data	2500	# of Training_data	1500	# of Training_data	2000	# of Training_data	1500

Table S2: Lattice thermal conductivity values and lattice constants for all considered materials.

Graphene		
	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Lattice Constants (Å)
DFT	3344.55	2.468
GAP	3469.88	2.468
DFT-HIPHIVE	3191.87	
GAP-HIPHIVE	3323.15	
Silicene		
	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Lattice Constants (Å)
DFT	33.87	3.868
GAP	34.76	3.872
DFT-HIPHIVE	33.96	
GAP-HIPHIVE	35.22	
***h*-BN**		
	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Lattice Constant (Å)
DFT	914.82	2.512
GAP	933.96	2.514
DFT-HIPHIVE	913.33	
GAP-HIPHIVE	872.84	
***h*-AlN**		
	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Lattice Constants (Å)
DFT	110.17	3.126
GAP	117.81	3.127

DFT-HIPHIVE	108.37	
GAP-HIPHIVE	113.35	
h-GaN		
	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Lattice Constants (Å)
DFT	44.95	3.255
GAP	44.65	3.256
DFT-HIPHIVE	43.41	
GAP-HIPHIVE	42.05	